Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ab initio calculations of the vibrational and dielectric properties of PbSnTe alloys LUISA SCOLFARO, Texas State University, USA, A.R. REZENDE NETO, H.W. LEITE ALVES, Universidade Federal de Sao Joao del Rei, Brazil, J.E. PETERSEN, T.H. MYERS, Texas State University, USA, P.D. BORGES, Universidade Federal de Viosa, Brazil — Thermoelectric devices have promise in dealing with the challenges of the growing demand for alternative clean energy and Te-based materials well-known candidates for them. Recently [1], we have shown that the high values for the dielectric constant, together with anharmonic LA-TO coupling, reduces the lattice thermal conductivity and enhances the electronic conductivity in PbTe. Also, it was shown that by alloying this material with Se, the electronic conductivity of the alloys is also enhanced [2]. But, it is not clear if the same occurs when alloying with Sn. We show, in this work, our ab initio results for the vibrational and dielectric properties of $Pb_{1-x}Sn_xTe$ alloys. The calculations were carried out by using the Density Functional Theory, and the alloys were described by both the Virtual Crystal Approximation and Cluster Expansion Method. Our results show that the anharmonic LA-TO coupling enhances and reach its maximum for Sn concentration values of 0.75, corresponding to the maximum value for the dielectric constant, which is higher than that obtained for PbTe. [1] H. W. Leite Alves, et al., Phys. Rev. B87, 115204 (2013). [2] Y. Pei, et al., Nature 473, 66 (2011).

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Date submitted: 06 Nov 2015 Electronic form version 1.4